

EFFECTIVE DIFFUSION IN THE REGION BETWEEN TWO SURFACES

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ABSTRACT. The purpose of this paper is to provide a formula for the effective diffusion operator \mathcal{D} obtained by projecting the 3-dimensional diffusion equation onto a 2-dimensional plane, assuming reflective boundary conditions at two surfaces in 3-dimensional space. The formula provided corresponds to the case of finite transversal stabilization rate in contrast to the infinite transversal stabilization rate formula provided in [8].

1. INTRODUCTION

The problem of understanding spatially constrained diffusion plays an important role in diverse areas such as biology, chemistry and nano-technology. Solving the diffusion equation for general constraining geometries is a very difficult task. One way to deal with this obstacle is to reduce the degrees of freedom of the problem by considering only the main directions of transport. More concretely, consider the diffusion equation

$$\frac{\partial P}{\partial t}(x, t) = D_0 \Delta P(x, t) \quad \text{where } x = (x_1, \dots, x_n)$$

with reflective boundary conditions in the border of the region of interest. By integrating this equation along adequate transversal directions to the main directions of transport, we obtain (in an approximate manner) a diffusion equation of the form

$$\frac{\partial p}{\partial t}(y, t) = \nabla \cdot (\mathcal{D}(y) \nabla p(y, t)) \quad \text{where } y = (y_1, \dots, y_m) \text{ and } m < n.$$

The $m \times m$ matrix $\mathcal{D}(y)$ in the above formula is known as *the effective diffusion matrix*, p is the *effective density function*, and $\nabla \cdot$ and ∇ are the divergence and gradient operators in an adequate metric in the y -variables (see [8]). The estimates of \mathcal{D} fall into two categories.

- (1) *Infinite transversal diffusion rate.* In this case it is assumed the the density function P stabilizes infinitely fast in directions transversal to the main directions of transport. In [8] we have given a very general formula for \mathcal{D} for arbitrary values of m and n with $m < n$. This formula contains as special cases the results in [6] and [2] given for $n = 3$ and $m = 1$.
- (2) *Finite transversal diffusion rate.* In this case it is assumed the the density function P stabilizes in finite time in directions transversal to the main

Effective diffusion matrix \mathcal{D}	Width function and fields
$\mathcal{D} = D_0 \begin{pmatrix} \omega & -\omega\mu \sin(\psi) \\ -\rho \sin(\psi) & \cos^2(\psi) + \mu\rho \sin^2(\psi) \end{pmatrix}$	$w = z_2 - z_1$
$\psi = \arcsin \left(\frac{\nabla z_1 \cdot \nabla^\perp z_2}{\sqrt{1+ \nabla z_1 ^2} \sqrt{1+ \nabla z_2 ^2}} \right)$	$\nabla w, \nabla^\perp w$
$m_i = \frac{\nabla z_i \cdot \nabla w}{(\nabla z_i \cdot \nabla^\perp w) \sin(\psi) + \nabla w \cos(\psi)}$	$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right)$ $\nabla^\perp = \left(-\frac{\partial}{\partial y}, \frac{\partial}{\partial x} \right)$
$\rho + i\omega = \left(\frac{1}{m_2 - m_1} \right) \log \left(\frac{1 + im_2}{1 + im_1} \right)$	
$\mu = \frac{m_1 + m_2}{2}$	

TABLE 1. Effective diffusion matrix \mathcal{D} for surfaces $z = z_1(x, y)$ and $z = z_2(x, y)$. The matrix is computed in the basis formed by the fields $\nabla w, \nabla^\perp w$.

directions of transport. This case has been studied extensively for $n = 2$ and $m = 1$ in articles like [9], [1], [7], [4].

In this article we provide a formula for the effective diffusion matrix in the finite transversal rate case, obtained by projecting the diffusion equation in x, y, z variables onto the x, y variables. We assume that reflective boundary conditions hold on the region bounded by surfaces of the form $z = z_1(x, y)$ and $z = z_2(x, y)$, where $z_1(x, y) < z_2(x, y)$. Our results are summarized in Table 1.

The outline of the article is as follows.

- In section 2 we recall the effective continuity equation and the effective diffusion matrix in the *infinite transversal rate case*, and explain the technique used in the next section to derive the formula for the effective diffusion matrix in the *finite transversal rate case*.
- In section 3 we compute a formula for the effective diffusion matrix \mathcal{D} in the finite transversal rate case for two planes in 3-dimensional space, and construct an effective diffusion ellipsoid $E_{\mathcal{D}}$ which will help us to understand the geometric and physical properties of \mathcal{D} .
- In section 4 we use the results in the the previous sections to compute a formula for the effective diffusion matrix (in the finite transversal rate case) for two surfaces of the form $z = z_1(x, y)$ and $z = z_2(x, y)$.
- In section 5 we apply our formula for \mathcal{D} to an specific examples. In particular, we recover the results in [3] (for channels in the plane) as a special case of our more general formula.

2. THE EFFECTIVE DIFFUSION EQUATION

Consider the region in 3-dimensional space given by the set of points (x, y, z) that satisfy

$$(2.1) \quad z_1(x, y) \leq z \leq z_2(x, y),$$

where $z_1 = z_1(x, y)$ and $z_2 = z_2(x, y)$ are scalar functions. We are interested in the *continuity equation*

$$(2.2) \quad \frac{\partial P}{\partial t} + D_0 \nabla \cdot \mathbf{J} = 0,$$

where $P = P(x, y, z, t)$ is the *concentration density* and $\mathbf{J} = \mathbf{J}(x, y, z, t)$ is the *density flux* vector field, with reflective boundary conditions

$$(2.3) \quad \mathbf{J}(x, y, z_i(x, y), t) \cdot \mathbf{n}_i(x, y) = 0$$

where the unit normal \mathbf{n}_i to the surface $z = z_i(x, y)$ is given by

$$\mathbf{n}_i = \frac{(-\nabla z_i, 1)}{\sqrt{1 + |\nabla z_i|^2}}.$$

The *effective concentration density* is given by

$$p(x, y, t) = \int_{z_1(x, y)}^{z_2(x, y)} P(x, y, z, t) dz$$

and the *effective density flux* by

$$(2.4) \quad \mathbf{j}(x, y, t) = (j_1(x, y, t), j_2(x, y, t)),$$

where for $\mathbf{J} = (J_1, J_2, J_3)$ we have that

$$j_i(x, y, t) = \int_{z_1(x, y)}^{z_2(x, y)} J_i(x, y, z) dz.$$

If the continuity equation 2.2 and the reflective boundary conditions 2.3 hold, we have the *effective continuity equation* (see [8])

$$(2.5) \quad \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{j} = 0.$$

We will assume that *Fick's law*, i.e

$$(2.6) \quad \mathbf{J} = -D_0 \nabla P,$$

for a constant scalar value D_0 , so that the continuity equation becomes the *diffusion equation*

$$(2.7) \quad \frac{\partial P}{\partial t} = D_0 \Delta P.$$

Infinitely transversal diffusion rate case. In this case P must be constant along the z -variable, i.e

$$P = P(x, y, t),$$

and the effective continuity equation 2.5 becomes (see [8])

$$\frac{\partial p}{\partial t}(x, y, t) = \nabla \cdot \left(w(x, y) \nabla \left(\frac{p(x, y, t)}{w(x, y)} \right) \right),$$

where the gradient and divergence operators in the above formula are given by

$$\nabla p = \left(\frac{\partial p}{\partial x}, \frac{\partial p}{\partial y} \right) \quad \text{and} \quad \nabla \cdot \mathbf{j} = \frac{\partial j_1}{\partial x} + \frac{\partial j_2}{\partial y},$$

which are the gradient and divergence operators in flat space. In [8] we showed that this equation can be written as a diffusion equation

$$(2.8) \quad \frac{\partial p}{\partial t}(x, y, t) = \nabla \cdot (\nabla p(x, y, t)),$$

if the divergence and gradient operators used are the ones associated to the metric tensor

$$(2.9) \quad g_w(x, y) = w(x, y) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

i.e

$$\begin{aligned} \nabla p &= \frac{1}{w} \left(\frac{\partial p}{\partial x}, \frac{\partial p}{\partial y} \right), \\ \nabla \cdot \mathbf{j} &= \frac{1}{w} \left(\frac{\partial}{\partial x}(w j_1) + \frac{\partial}{\partial y}(w j_2) \right). \end{aligned}$$

A consequence of this is that we can study the effective diffusion equation 2.8 by simulating random walks with steps constructed using geodesic segments of the metric g_w .

Finetely transversal diffusion rate case. We are looking for a matrix-valued function $\mathcal{D} = \mathcal{D}(x, y)$ such that the projection of the diffusion process in the x, y -plane is modeled by an equation of the form

$$\frac{\partial p}{\partial t}(x, y, t) = \nabla \cdot (\mathcal{D}(x, y) \nabla p(x, y, t)),$$

where the gradient and divergence operators $\nabla \cdot$ and ∇ are the ones associated with the metric tensor 2.9.

To compute \mathcal{D} we consider harmonic functions $Q = Q(x, y, z)$ (i.e stable solutions of the diffusion equation) satisfying reflective boundary conditions in the region of interest. If Fick's law holds, i.e

$$\mathbf{J}_Q = -D_0 \left(\frac{\partial Q}{\partial x}, \frac{\partial Q}{\partial y}, \frac{\partial Q}{\partial z} \right),$$

the effective density and flux are given by

$$\begin{aligned} q &= \int_{z_1}^{z_2} Q dz, \\ j_Q &= -D_0 \left(\int_{z_1}^{z_2} \frac{\partial Q}{\partial x} dz, \frac{\partial}{\partial y} \int_{z_1}^{z_2} \frac{\partial Q}{\partial y} dz \right). \end{aligned}$$

We can then compute \mathcal{D} from the formula (see [5])

$$j_Q = -w \mathcal{D} \left(\nabla \left(\frac{q}{w} \right) \right),$$

to obtain

$$(2.10) \quad \mathcal{D} \left(\nabla \left(\frac{q}{w} \right) \right) = \frac{D_0}{w} \left(\int_{z_1}^{z_2} \frac{\partial Q}{\partial x} dz, \int_{z_1}^{z_2} \frac{\partial Q}{\partial y} dz \right).$$

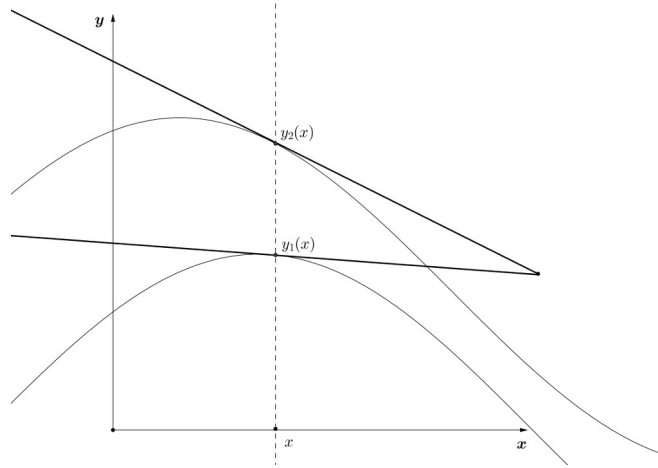
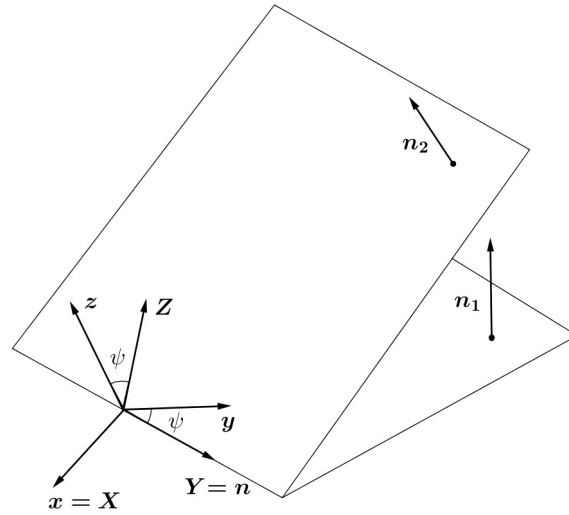


FIGURE 2.1. Approximation of a channel by an angular sector

FIGURE 3.1. Intersecting planes and ortho-normal basis $\mathbf{x}, \mathbf{y}, \mathbf{z}$.

In general it is not always possible to find explicit formulas for harmonic functions Q with the required boundary conditions. In such cases we approximate the region of interest with a simpler one in which we can find such functions (see Figure 2.1)

3. EFFECTIVE DIFFUSION MATRIX FOR TWO PLANES

Consider two planes with non-parallel normal vectors $\mathbf{n}_1, \mathbf{n}_2$ and let \mathbf{z} be the unit vector along the direction of projection. The intersection of the planes is spanned by the unit vector

$$\mathbf{n} = \frac{\mathbf{n}_1 \times \mathbf{n}_2}{|\mathbf{n}_1 \times \mathbf{n}_2|}.$$

Consider the ortho-normal basis (see Figure 3.1)

$$(3.1) \quad \mathbf{x} = \frac{\mathbf{n} \times \mathbf{z}}{|\mathbf{n} \times \mathbf{z}|}, \mathbf{y} = \mathbf{z} \times \mathbf{x} \text{ and } \mathbf{z}.$$

and denote the coordinates in this basis by x, y and z . Since \mathbf{n} is unitary and orthogonal to \mathbf{x} we can write

$$\mathbf{n} = \cos(\psi)\mathbf{y} + \sin(\psi)\mathbf{z},$$

where the angle ψ , which we will refer to as the *tilt*, is given by

$$(3.2) \quad \psi = \arcsin(\mathbf{n} \cdot \mathbf{z}) \text{ and } -\frac{\pi}{2} \leq \psi \leq \frac{\pi}{2}.$$

The tilt is simply the angle that the intersection line of the two planes forms with the projection plane. If X, Y and Z are the coordinates in the frame

$$\begin{aligned} \mathbf{X} &= \mathbf{x}, \\ \mathbf{Y} = \mathbf{n} &= \cos(\psi)\mathbf{y} + \sin(\psi)\mathbf{z}, \\ \mathbf{Z} &= -\sin(\psi)\mathbf{y} + \cos(\psi)\mathbf{z}. \end{aligned}$$

then we have that

$$\begin{aligned} X &= x, \\ Y &= y \cos(\psi) + z \sin(\psi), \\ Z &= -y \sin(\psi) + z \cos(\psi). \end{aligned}$$

Using these coordinates we can construct a family of functions (parametrized by $0 \leq \omega < 2\pi$) as follows

$$Q_\omega = \cos(\omega) \log(X^2 + Z^2)/2 + \sin(\omega)Y.$$

By construction

$$\begin{aligned} Q_0 &= \log(X^2 + Z^2) \\ Q_{\frac{\pi}{2}} &= Y \end{aligned}$$

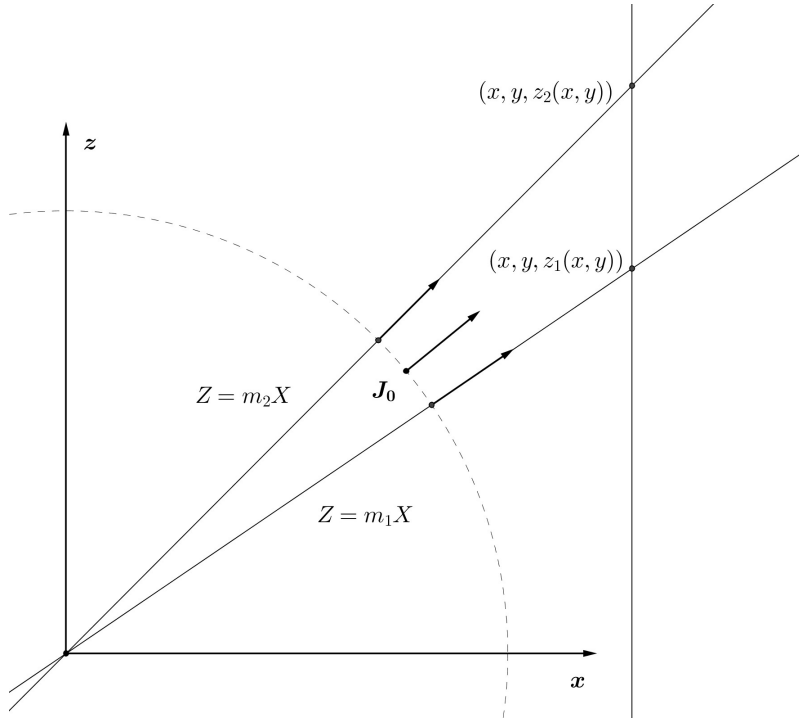
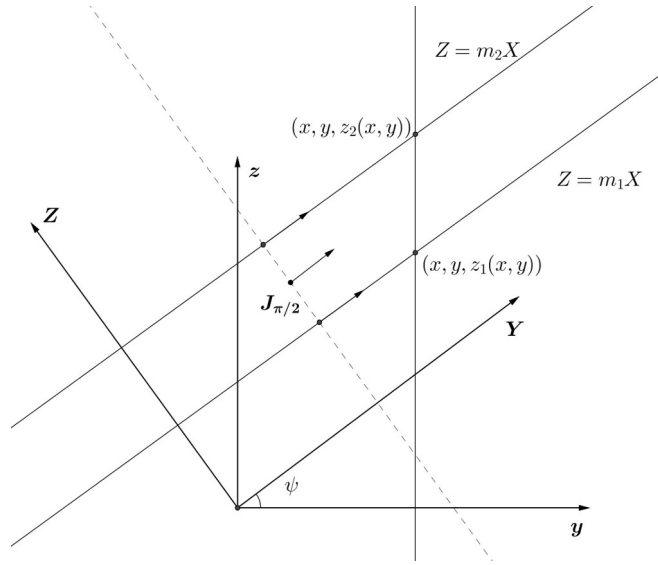
are harmonic functions satisfying reflective boundary conditions with respect to the planes with normal vectors \mathbf{n}_1 and \mathbf{n}_2 (see Figures 3.2 and 3.3), and hence so it is Q_ω for all $0 \leq \omega < 2\pi$.

Computing the effective diffusion operator. We have that

$$\begin{aligned} \frac{\partial Q_\omega}{\partial x} &= \frac{X \cos(\omega)}{x^2 + Z^2} \\ \frac{\partial Q_\omega}{\partial y} &= \cos(\psi) \sin(\omega) - \frac{Z \sin(\psi) \cos(\omega)}{x^2 + Z^2}, \end{aligned}$$

and hence

$$\begin{aligned} \int_{z_1}^{z_2} \frac{\partial Q_\omega}{\partial x} dz &= [\arctan(Z/x) \sec(\psi) \cos(\omega)]_{z=z_1}^{z=z_2}, \\ \int_{z_1}^{z_2} \frac{\partial Q_\omega}{\partial y} dz &= \left[z \cos(\psi) \sin(\omega) - \frac{1}{2} \log(x^2 + Z^2) \tan(\psi) \cos(\omega) \right]_{z=z_1}^{z=z_2}. \end{aligned}$$

FIGURE 3.2. Flow J_0 of $P_0 = \log(X^2 + Y^2)$ FIGURE 3.3. Flow $J_{\frac{\pi}{2}}$ of $P_{\frac{\pi}{2}} = Y$.

The functions z_i 's are obtained by solving the equation $Z = m_i X$ (see Figures 3.2 and 3.3), which gives us

$$z_i = (m_i x + y \sin(\psi)) \sec(\psi),$$

where

$$(3.3) \quad m_i = -\frac{\mathbf{n}_i \cdot \mathbf{X}}{\mathbf{n}_i \cdot \mathbf{Z}} = \frac{\mathbf{n}_i \cdot \mathbf{x}}{(\mathbf{n}_i \cdot \mathbf{y}) \sin(\psi) - (\mathbf{n}_i \cdot \mathbf{z}) \cos(\psi)}$$

From the above equations we obtain that

$$\int_{z_1}^{z_2} \frac{\partial Q_\omega}{\partial x} dz = (\arctan(m_2) - \arctan(m_1)) \sec(\psi) \cos(\omega)$$

and

$$\begin{aligned} \int_{z_1}^{z_2} \frac{\partial Q_\omega}{\partial x} dz &= (m_2 - m_1) x \sin(\omega) \\ &- \log \left(\frac{\sqrt{1+m_2^2}}{\sqrt{1+m_1^2}} \right) \tan(\psi) \cos(\omega). \end{aligned}$$

If we let

$$(v_{\omega,1}, v_{\omega,2}) = \nabla \left(\frac{q_\omega(x, y)}{w(x, y)} \right)$$

then

$$\begin{aligned} v_{\omega,1} &= \left(\frac{m_1 + m_2}{2} \right) \sin(\omega) \tan(\psi) + \cos(\omega)/x, \\ v_{\omega,2} &= \sec(\psi) \sin(\omega). \end{aligned}$$

We want to solve (for \mathcal{D}) the equation

$$\mathcal{D} \begin{pmatrix} v_{\omega,1} \\ v_{\omega,2} \end{pmatrix} = \begin{pmatrix} j_{\omega,1} \\ j_{\omega,2} \end{pmatrix}.$$

Since this must hold for all ω 's it must hold in particular for $\omega = 0$ and $\omega = \pi/2$, i.e

$$(3.4) \quad \mathcal{D} = \begin{pmatrix} \mathcal{D}_{11} & \mathcal{D}_{12} \\ \mathcal{D}_{21} & \mathcal{D}_{22} \end{pmatrix} = \begin{pmatrix} j_{0,1} & j_{\frac{\pi}{2},1} \\ j_{0,2} & j_{\frac{\pi}{2},2} \end{pmatrix} \begin{pmatrix} v_{0,1} & v_{\frac{\pi}{2},1} \\ v_{0,2} & v_{\frac{\pi}{2},2} \end{pmatrix}^{-1},$$

which implies that

$$\mathcal{D} = \begin{pmatrix} \mathcal{D}_{11} & \mathcal{D}_{12} \\ \mathcal{D}_{21} & \mathcal{D}_{11} \end{pmatrix},$$

where

$$\begin{aligned} \mathcal{D}_{11} &= D_0 \left(\frac{\arctan(m_2) - \arctan(m_1)}{m_2 - m_1} \right) \\ \mathcal{D}_{12} &= -D_0 \left(\frac{\arctan(m_2) - \arctan(m_1)}{m_2 - m_1} \right) \left(\frac{m_1 + m_2}{2} \right) \sin(\psi), \\ \mathcal{D}_{21} &= -D_0 \left(\frac{\sin(\psi)}{m_2 - m_1} \right) \log \left(\frac{\sqrt{1+m_2^2}}{\sqrt{1+m_1^2}} \right), \\ \mathcal{D}_{22} &= D_0 \left(\cos^2(\psi) + \frac{1}{2} \left(\frac{m_1 + m_2}{m_2 - m_1} \right) \log \left(\frac{\sqrt{1+m_2^2}}{\sqrt{1+m_1^2}} \right) \sin^2(\psi) \right). \end{aligned}$$

We can write the matrix of \mathcal{D} more compactly as

$$\mathcal{D} = D_0 \begin{pmatrix} \omega & -\omega\mu \sin(\psi) \\ -\rho \sin(\psi) & \cos^2(\psi) + \mu\rho \sin^2(\psi) \end{pmatrix},$$

where

$$\rho + i\omega = \left(\frac{1}{m_2 - m_1} \right) \log \left(\frac{1 + im_2}{1 + im_1} \right) \quad \text{and} \quad \mu = \frac{1}{2}(m_1 + m_2).$$

Remark. Recall the the complex logarithm function is defined by

$$\log(x + iy) = \log(\sqrt{x^2 + y^2}) + i \arctan(y/x).$$

The scalars \mathcal{D}_{ij} 's are the coefficients of the linear operator \mathcal{D} in the ortho-normal frame formed by \mathbf{x} and \mathbf{y} , i.e

$$(3.5) \quad \mathcal{D}(\mathbf{x}) = \mathcal{D}_{11}\mathbf{x} + \mathcal{D}_{12}\mathbf{y},$$

$$(3.6) \quad \mathcal{D}(\mathbf{y}) = \mathcal{D}_{21}\mathbf{x} + \mathcal{D}_{22}\mathbf{y}.$$

The diffusion ellipsoid and principal response lines. Consider a square matrix A with real coefficients and $\det(A) \neq 0$. The matrix

$$S_A = (AA^T)^{1/2}$$

is well defined since AA^T is symmetric and positive definite. If we let

$$R_A = S_A^{-1}A$$

then we can write

$$A = S_A R_A,$$

where the matrix R_A is orthogonal (since $R_A R_A^T = S_A^{-1} A A^T S_A^{-1} = I$). In words, any square matrix is the product of a symmetric matrix and an orthogonal one.

If we apply the above result to \mathcal{D} we obtain the decomposition

$$\mathcal{D} = S_{\mathcal{D}} R_{\mathcal{D}}.$$

Hence, the circle of unit vectors maps under \mathcal{D} to an ellipsoid $E_{\mathcal{D}}$ having its mayor and minor axes aligned with the eigen-vectors of $S_{\mathcal{D}}$ and the corresponding widths are given by the eigenvalues of $S_{\mathcal{D}}$. We will refer to $E_{\mathcal{D}}$ as the *effective diffusion ellipsoid*. For unit vectors $\mathbf{f}_{\mathcal{D},1}$ and $\mathbf{f}_{\mathcal{D},2}$ aligned with the mayor and minor axes of $E_{\mathcal{D}}$ the unit vectors $\mathbf{e}_{\mathcal{D},1} = R_{\mathcal{D}}^T \mathbf{f}_1$ and $\mathbf{e}_{\mathcal{D},2} = R_{\mathcal{D}}^T \mathbf{f}_2$ map under the action of \mathcal{D} to vectors whose end points lay in $E_{\mathcal{D}}$ and aligned with its mayor and minor axes (see Figure 3.4). We will refer to the lines spanned by $\mathbf{e}_{\mathcal{D},1}, \mathbf{e}_{\mathcal{D},2}$ as *principal response lines* of \mathcal{D} . The physical meaning of these lines can be obtained by recalling Fick's formula

$$\mathbf{j} = -\mathcal{D} \nabla p,$$

so that when ∇p is aligned with $\mathbf{e}_{\mathcal{D},1}$ the corresponding relative flux magnitude $|\mathbf{j}|/|\nabla p|$ is maximal. Similarly, when ∇p is aligned with $\mathbf{e}_{\mathcal{D},2}$ the value of $|\mathbf{j}|/|\nabla p|$ is minimal.

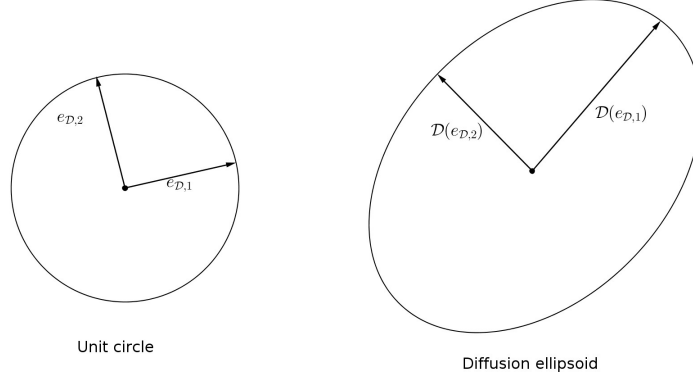


FIGURE 3.4. Principal response directions

The case of parallel planes. In this case $\mathbf{n}_1 = \mathbf{n}_2$, which implies that $m_1 = m_2 = \mu$. In particular, the vector

$$\mathbf{n} = \frac{\mathbf{n}_1 \times \mathbf{n}_2}{|\mathbf{n}_1 \times \mathbf{n}_2|}$$

is not well defined and can not be used to construct the frame \mathbf{x}, \mathbf{y} (see 3.1). Instead, for

$$\mathbf{n}_1 = \mathbf{n}_2 = (a, b, c)$$

we let

$$\mathbf{n} = \begin{cases} \frac{1}{\sqrt{a^2+b^2}}(-b, a, 0) & \text{if } a^2 + b^2 > 0, \\ (0, 1, 0) & \text{if } a^2 + b^2 = 0. \end{cases}$$

so that for $a^2 + b^2 > 0$ we get

$$\mathbf{x} = \frac{1}{\sqrt{a^2+b^2}}(a, b, 0), \mathbf{y} = \frac{1}{\sqrt{a^2+b^2}}(-b, a, 0)$$

and for $a^2 + b^2 = 0$ we get

$$\mathbf{x} = (1, 0, 0) \text{ and } \mathbf{y} = (0, 1, 0).$$

In both cases we have that $\psi = 0$ (see 3.2) and since

$$\begin{aligned} \rho + i\omega &= \lim_{m_1, m_2 \rightarrow \mu} \left(\frac{1}{m_2 - m_1} \right) \log \left(\frac{1 + im_2}{1 + im_1} \right), \\ &= \frac{d}{d\mu} (\log(1 + i\mu)) = \frac{i}{1 + i\mu} \\ &= \frac{\mu + i}{1 + \mu^2}, \end{aligned}$$

we obtain

$$(3.7) \quad \mathcal{D} = D_0 \begin{pmatrix} \frac{1}{1+\mu^2} & 0 \\ 0 & 1 \end{pmatrix},$$

where μ is the common slope of the two planes with respect to the x, y -plane. When $\mu = 0$ the planes are parallel to the x, y -plane and the effective diffusion operator

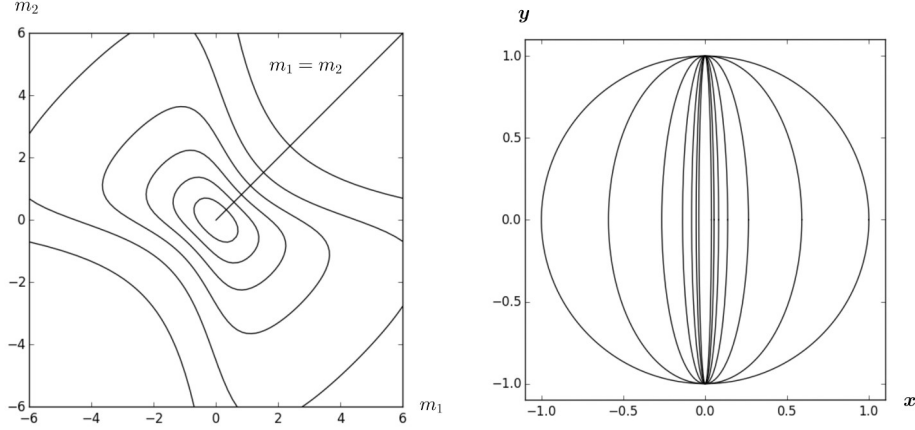


FIGURE 3.5. Effective diffusion ellipsoids for $\psi = 0$ and $D_0 = 1$. Each level curve of ω (left) corresponds to a single ellipsoid (right). As we move along the ray $m_1 = m_2 = \mu \geq 0$ we obtain ellipsoids with semi-axis $1/(1 + \mu^2)$ and 1.

is simply scalar multiplication by D_0 , i.e the diffusion equation remains unchanged after the projection procedure. This is to be expected, as in this case the walls have no effect on the diffusion process in the main direction of transport.

The case of non-parallel planes with no tilt. In this case we have $m_1 \neq m_2$ and $\psi = 0$, i.e the two planes are non-parallel and their intersection line is parallel to the x, y -plane. We then have that

$$(3.8) \quad \mathcal{D} = D_0 \begin{pmatrix} \omega & 0 \\ 0 & 1 \end{pmatrix},$$

where

$$\omega = \frac{\arctan(m_2) - \arctan(m_1)}{m_2 - m_1}.$$

Observe that when $m_1 = m_2$ formula 3.8 becomes 3.7.

The effective diffusion ellipsoid $E_{\mathcal{D}}$ has \mathbf{x} and \mathbf{y} as principal axes and corresponding widths $D_0\omega$ and D_0 . The dependence of $E_{\mathcal{D}}$ on m_1 and m_2 is shown in Figure 3.5.

The case of extreme tilts. This occurs when $\psi = -\pi/2$ or $\psi = \pi/2$, i.e the planes are orthogonal to the x, y -plane, and we have corresponding diffusion matrices

$$\mathcal{D}_- = D_0 \begin{pmatrix} \omega & \mu\omega \\ \rho & \mu\rho \end{pmatrix} \quad \text{or} \quad \mathcal{D}_+ = D_0 \begin{pmatrix} \omega & -\mu\omega \\ -\rho & \mu\rho \end{pmatrix}.$$

Both matrices share the same eigen-values, given by

$$0, D_0(\mu\rho + \omega).$$

The eigen-vectors of \mathcal{D}_- are

$$(\mu, -1) \quad \text{and} \quad (\omega, \rho),$$

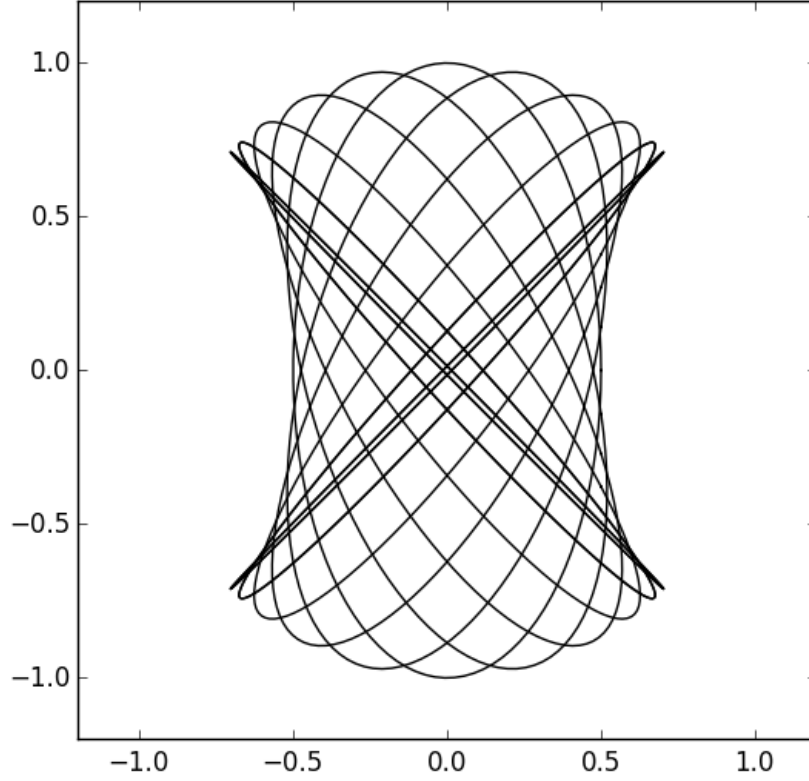


FIGURE 3.6. Effective diffusion ellipsoids obtained by varying the tilt parameter

and those of \mathcal{D}_+ are

$$(\mu, 1) \text{ and } (\omega, -\rho).$$

If $E_- = E_{\mathcal{D}_-}$ and $E_+ = E_{\mathcal{D}_+}$ then E_- is a line segment (a degenerate ellipsoid) joining the diametrically opposite points

$$\pm D_0 \left(\frac{\mu\rho + \omega}{(\omega^2 + \rho^2)^{1/2}} \right) (\omega, \rho)$$

and E_+ is a line segment joining the diametrically opposite points

$$\pm D_0 \left(\frac{\mu\rho + \omega}{(\omega^2 + \rho^2)^{1/2}} \right) (\omega, -\rho).$$

The case of varying tilt. If we vary the tilt parameter $-\pi/2 < \psi < \pi/2$ the effective diffusion ellipsoid gives us a family of ellipsoids which in the limiting cases $\psi = -\pi/2, \pi/2$ become line segments (see Figure 3.6)

4. THE EFFECTIVE DIFFUSION MATRIX FOR TWO SURFACES

For surfaces defined by $z = z_i(x, y)$ we chose their unit normal vectors as

$$\mathbf{n}_1 = -\frac{(-\nabla z_1, 1)}{\sqrt{1 + |\nabla z_1|^2}} \text{ and } \mathbf{n}_2 = \frac{(-\nabla z_2, 1)}{\sqrt{1 + |\nabla z_2|^2}},$$

where the signs are so that \mathbf{n}_1 and \mathbf{n}_2 point the outside of the region defined by the formula $z_1(x, y) \leq z_2(x, y)$. We then have that

$$\mathbf{n} = \mathbf{n}_1 \times \mathbf{n}_2 = \frac{(\nabla^\perp w, \nabla z_1 \cdot \nabla^\perp z_2)}{\sqrt{1 + |\nabla z_1|^2} \sqrt{1 + |\nabla z_2|^2}},$$

where the width function w is given by

$$w = z_2 - z_1,$$

and the operators ∇ and ∇^\perp are given by

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right) \quad \text{and} \quad \nabla^\perp = \left(-\frac{\partial}{\partial y}, \frac{\partial}{\partial x} \right).$$

We will refer to ∇^\perp as the *orthogonal gradient operator* (observe that $\nabla^\perp w$ is the Hamiltonian vector field of w). For $\mathbf{z} = (0, 0, 1)$ we have that

$$\mathbf{x} = \frac{\mathbf{n} \times \mathbf{z}}{|\mathbf{n} \times \mathbf{z}|} = \left(\frac{\nabla w}{|\nabla w|}, 0 \right) \quad \text{and} \quad \mathbf{y} = \mathbf{z} \times \mathbf{x} = \left(\frac{\nabla^\perp w}{|\nabla^\perp w|}, 0 \right).$$

Since \mathbf{x} and \mathbf{y} are in the plane $z = 0$ we will simply write

$$(4.1) \quad \mathbf{x} = \frac{\nabla w}{|\nabla w|} \quad \text{and} \quad \mathbf{y} = \frac{\nabla^\perp w}{|\nabla^\perp w|}.$$

Formulas 3.5 and 3.6 imply that

$$\begin{aligned} \mathcal{D}(\nabla w) &= \mathcal{D}_{11} \nabla w + \mathcal{D}_{12} \nabla^\perp w, \\ \mathcal{D}(\nabla^\perp w) &= \mathcal{D}_{21} \nabla w + \mathcal{D}_{22} \nabla^\perp w. \end{aligned}$$

We now compute m_1, m_2 and ψ , since we need them to compute the coefficients \mathcal{D}_{ij} 's. Using the formulas 4.1, 3.2 and 3.3 we obtain

$$(4.2) \quad \psi = \arcsin \left(\frac{\nabla z_1 \cdot \nabla^\perp z_2}{\sqrt{1 + |\nabla z_1|^2} \sqrt{1 + |\nabla z_2|^2}} \right).$$

and

$$(4.3) \quad m_i = \frac{\nabla z_i \cdot \nabla w}{(\nabla z_i \cdot \nabla^\perp w) \sin(\psi) + |\nabla w| \cos(\psi)}.$$

5. EXAMPLES

Recovering the 2-dimensional case. We assume that z_1 and z_2 are only functions of the x -variable and write $z_i = z_i(x)$, so that

$$\nabla z_i = (z'_i, 0).$$

This implies that the vectors $\nabla z_1, \nabla z_2$ and ∇w are all parallel, that the tilt ψ is identically zero and that

$$m_i = \frac{z'_i(z'_2 - z'_1)}{|z'_2 - z'_1|} = \pm z'_i,$$

where the plus sign is chosen at the points (x, y) where $z'_2 > z'_1$ (i.e $w' > 0$) and the minus sign at the points (x, y) where $z'_2 < z'_1$ (i.e $w' < 0$). We conclude that (irrespective of the sign in the above formula) \mathcal{D} is given by

$$(5.1) \quad \mathcal{D} = D_0 \begin{pmatrix} \frac{\arctan(z'_2) - \arctan(z'_1)}{z'_2 - z'_1} & 0 \\ 0 & 1 \end{pmatrix}.$$

The above formula for \mathcal{D} is its representations in basis formed by ∇w and $\nabla^\perp w$, but it is easy to see that in this case the same matrix represents \mathcal{D} in the basis formed by the vectors $(1, 0)$ and $(0, 1)$. Hence, we have obtained the result in [3] as a particular case of our formula for surfaces.

Remark. At the points (x, y) where $z'_2 = z'_1$ (i.e $w' = 0$) we have that

$$\mathcal{D} = \begin{pmatrix} \frac{1}{1+(z'_1)^2} & 0 \\ 0 & 1 \end{pmatrix}$$

Surfaces with vanishing tilt function. The tilt function ψ vanishes if ∇z_1 and ∇z_2 are parallel vectors at all points. This holds if we can write

$$z_i(x, y) = f_i(z(x, y)),$$

and in this case we have that

$$\nabla z_i = f'_i \nabla z \quad \text{and} \quad \nabla w = (f'_2 - f'_1) \nabla z.$$

Using formula 4.3 and assuming $f'_1 \neq f'_2$ we obtain

$$(5.2) \quad m_i = \pm f'_i |\nabla z|,$$

where the plus sign is selected if $f'_2 < f'_1$ and the minus sign if $f'_2 > f'_1$. We can then write

$$\mathcal{D} = D_0 \begin{pmatrix} \omega & 0 \\ 0 & 1 \end{pmatrix}$$

where (and independently of the choice of sign in formula 5.2) we have that

$$\omega = \frac{\arctan(f'_2 |\nabla z|) - \arctan(f'_1 |\nabla z|)}{(f'_2 - f'_1) |\nabla z|},$$

at the points (x, y) at which $f'_1 \neq f'_2$, and

$$\omega = \frac{1}{1 + (f'_1 |\nabla z|)^2} = \frac{1}{1 + (f'_2 |\nabla z|)^2}$$

at the points (x, y) where $f'_1 = f'_2$.

For example, if we let

$$z_1 = \sin(\sqrt{x^2 + y^2}) - 3/2 \quad \text{and} \quad z_2 = \cos(2\sqrt{x^2 + y^2}) + 3/2,$$

then

$$f_1 = \sin(r) - 3/2, f_2 = \cos(2r) + 3/2 \quad \text{and} \quad r = \sqrt{x^2 + y^2}.$$

In this case the integral curves of ∇w generate rays of the form

$$r \mapsto r(\cos(\theta), \sin(\theta)) \quad \text{where} \quad r \geq 0$$

and those of $\nabla^\perp w$ generate circles of the form

$$\theta \mapsto r(\cos(\theta), \sin(\theta)) \quad \text{where} \quad 0 \leq \theta < 2\pi.$$

Along the directions of the circles the diffusion process has effective diffusion constant equal to D_0 , and along the direction defined by the rays the diffusion process has effective diffusion function $D_0 \omega$ (see Figure 5.1) .

Remark. Observe that in this case the matrix \mathcal{D} is diagonal. Hence the principal response lines are generated by the vector fields $\nabla^\perp w$ and ∇w .

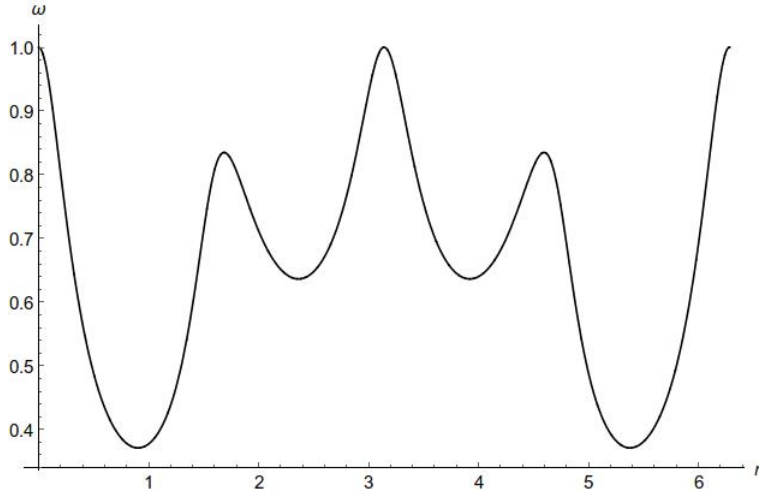


FIGURE 5.1. Radial effective diffusion function of the surfaces $z_1 = \sin(\sqrt{x^2 + y^2}) - 3/2$ and $z_2 = \cos(2\sqrt{x^2 + y^2}) + 3/2$.

An example with non-vanishing tilt function. Consider the orthogonal planar wave surfaces given by the functions

$$z_1 = \cos(x) \quad \text{and} \quad z_2 = \cos(y) + 5/2.$$

The tilt function is given by (see Figure 5.2)

$$\psi = -\arcsin\left(\frac{\sin(x)\sin(y)}{\sqrt{(1+\sin(x)^2)(1+\sin(y)^2)}}\right),$$

which only vanishes on the lines $x = n\pi$ and $y = m\pi$ for any integers m and n .

Recall that we have a decomposition of \mathcal{D} of the form

$$\mathcal{D} = S_{\mathcal{D}} R_{\mathcal{D}}$$

where $S_{\mathcal{D}}$ is symmetric and $R_{\mathcal{D}}$ is orthogonal. The eigenvalue functions λ_1 and λ_2 of $S_{\mathcal{D}}$ are shown in figure 5.3. In Figure 5.4 we show the gradient fields ∇w and $\nabla^\perp w$ of the width function $w = z_2 - z_1$, and the fields of principal directions of \mathcal{D} . In this case $\nabla^\perp w$ and ∇w do not in general span the principal responses lines, since the tilt function does not vanishes at all points.

6. CONCLUSIONS AND FUTURE WORK

We have obtained the effective diffusion matrix which results of projecting a diffusion process between two surfaces (of the form $z = z_1(x, y)$ and $z_2(x, y)$) onto the x, y -plane. In future work we plan to project the diffusion process into the middle surface $z_{1/2} = (z_1 + z_2)/2$, where we expect to obtain a more clear understanding of the effective diffusion operator. The added complication is that the differential geometry of the middle surface is now non-trivial, in contrast to the x, y -plane which is a flat.

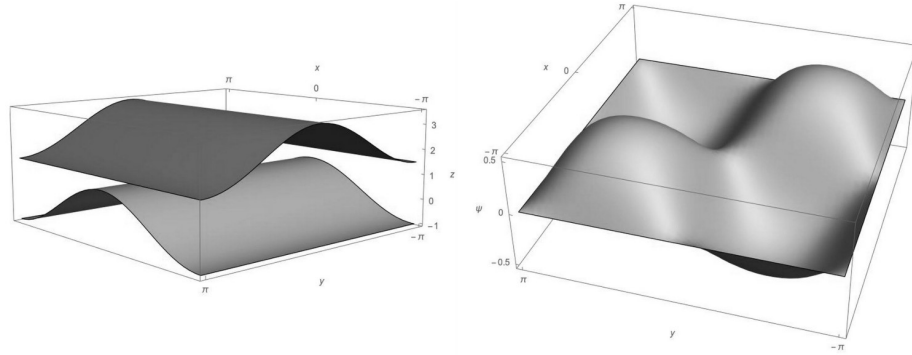


FIGURE 5.2. Two orthogonal planar waves (left) and their tilt function (right)

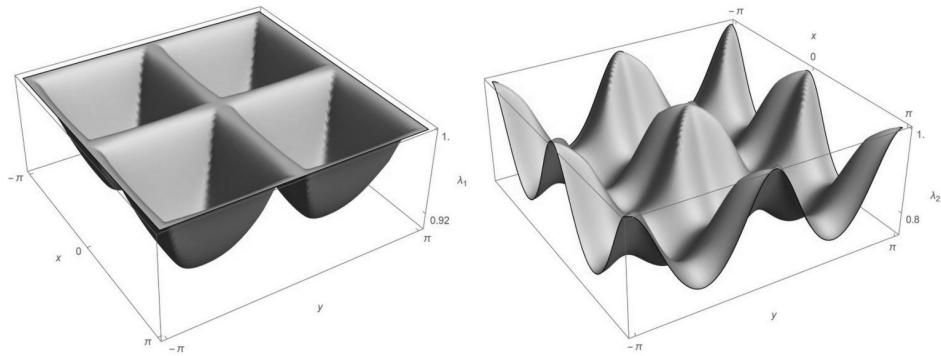


FIGURE 5.3. Eigenvalue functions of two planar orthogonal waves

7. AKNOWLEDGMENTS

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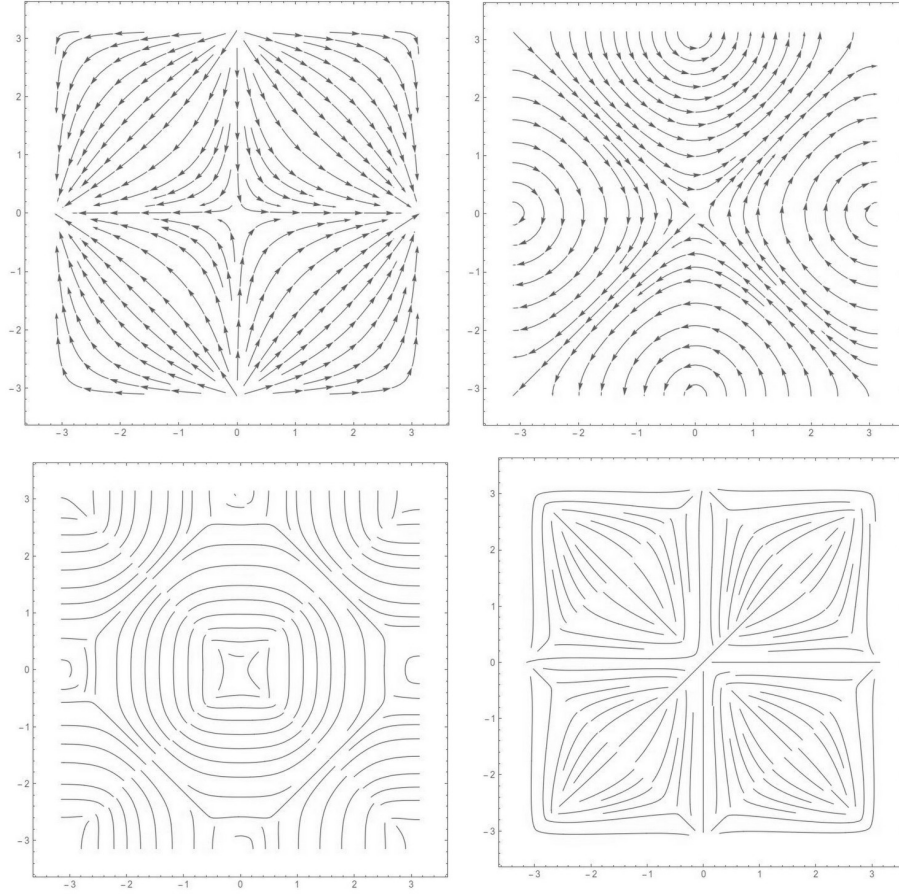


FIGURE 5.4. Vector and line fields of two orthogonal wave-like functions. The vector fields ∇w (upper left corner) and $\nabla^\perp w$ (upper right corner), and the line fields spanned by $e_{\mathcal{D},1}$ (lower left corner) and $e_{\mathcal{D},2}$ (lower right corner).

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